SI Table ---:

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| --- | --- | --- | --- |
| Complex | Global heavy atom RMSD | Co-factor loop RMSD | Substrate RMSD |
| 4FVT (ternary complex) – Xtal vs 4BVG ( native intermediate) Xtal | 0.5 Å | 4.0 Å | NAD part (0.8 Å)  peptide  (0.3 Å) |
| 4FVT (ternary complex) – Xtal  vs  4FVT (ternary complex) – MD averaged | 1.1Å | 2.2Å | NAD part (0.4Å)  Peptide part  (1 Å) |
| 4BVG (native intermediate) Xtal  vs  4BVG (native intermediate) MD averaged | 1.6Å | 1.8Å | NAD (0.5Å)  Peptide part  ( 2.6 Å) |
| 3GLS (apo Sirt3) – Xtal  vs  3GLS (apo Sirt3) – MD averaged | 1.1Å | 0.79Å | Not applicable |
| Sirt3/ADPR complex/NAM modelled from 4FVT (**MD average**)  vs  Sirt3/ADPR complex/NAM modelled from 4FVT but with loop replaced form 4BVG (**MD average**) | 2.2 Å | 5.9Å | NAD (0.4Å)  Peptide part  ( 0.9Å)  NAM  (6.7 Å) |
| 4FVT (ternary complex) – Xtal  vs  Sirt3/ADPR complex/NAM modelled from 4FVT (MD average) | 1.9Å | 3.9Å | NAD part (0.62Å)  peptide part  ( 0.5Å) |
| 4FVT (ternary complex) – Xtal  vs  Sirt3/ADPR complex/NAM modelled from 4FVT but with loop replaced form 4BVG (MD average) | 1.1Å | 3.7Å | NAD part (0.3Å)  peptide part  (0.7 Å) |
| 4BVG (native intermediate) Xtal  vs  Sirt3/ADPR complex/NAM modelled from 4FVT (MD average) | 2.0Å | 6.3Å | NAD part (0.65.Å)  peptide part  ( 0.55Å) |
| 4BVG (native intermediate) Xtal  vs  Sirt3/ADPR complex/NAM modelled from 4FVT but with loop replaced form 4BVG (MD average) | 1.0Å | 1.4Å | NAD part (0.4.Å)  peptide part  ( 0.8Å) |

*\*Note: Only the matching atoms were considered for RMSD calculation.*